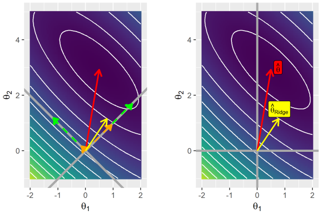
Introduction to Machine Learning

Regularization
Geometry of L2 Regularization



Learning goals

- Approximate transformation of unregularized minimizer to regularized
- Principal components of Hessian influence where parameters are decayed

GEOMETRIC ANALYSIS OF $L2$ REGULARIZATION

Quadratic Taylor approx of the unregularized objective $\mathcal{R}_{\text{emp}}(\boldsymbol{\theta})$ around its minimizer $\hat{\boldsymbol{\theta}}$:

$$\tilde{\mathcal{R}}_{\text{emp}}(\boldsymbol{\theta}) = \mathcal{R}_{\text{emp}}(\hat{\boldsymbol{\theta}}) + \nabla_{\boldsymbol{\theta}} \mathcal{R}_{\text{emp}}(\hat{\boldsymbol{\theta}}) \cdot (\boldsymbol{\theta} - \hat{\boldsymbol{\theta}}) + \frac{1}{2}(\boldsymbol{\theta} - \hat{\boldsymbol{\theta}})^T \boldsymbol{H}(\boldsymbol{\theta} - \hat{\boldsymbol{\theta}})$$

where $\boldsymbol{H}$ is the Hessian of $\mathcal{R}_{\text{emp}}(\boldsymbol{\theta})$ at $\hat{\boldsymbol{\theta}}$

We notice:

- First-order term is 0, because gradient must be 0 at minimizer
- $\boldsymbol{H}$ is positive semidefinite, because we are at the minimizer

$$\tilde{\mathcal{R}}_{\text{emp}}(\boldsymbol{\theta}) = \mathcal{R}_{\text{emp}}(\hat{\boldsymbol{\theta}}) + \frac{1}{2}(\boldsymbol{\theta} - \hat{\boldsymbol{\theta}})^T \boldsymbol{H}(\boldsymbol{\theta} - \hat{\boldsymbol{\theta}})$$

GEOMETRIC ANALYSIS OF $L2$ REGULARIZATION / 2

The minimum of $\tilde{\mathcal{R}}_{\text{emp}}(\boldsymbol{\theta})$ occurs where $\nabla_{\boldsymbol{\theta}}\tilde{\mathcal{R}}_{\text{emp}}(\boldsymbol{\theta}) = \boldsymbol{H}(\boldsymbol{\theta} - \hat{\boldsymbol{\theta}})$ is 0.
Now we $L2$-regularize $\tilde{\mathcal{R}}_{\text{emp}}(\boldsymbol{\theta})$, such that

$$\tilde{\mathcal{R}}_{\text{reg}}(\boldsymbol{\theta}) = \tilde{\mathcal{R}}_{\text{emp}}(\boldsymbol{\theta}) + \frac{\lambda}{2}\|\boldsymbol{\theta}\|_2^2$$

and solve this approximation of $\mathcal{R}_{\text{reg}}$ for the minimizer $\hat{\boldsymbol{\theta}}_{\text{ridge}}$:

$$\begin{aligned}
\nabla_{\boldsymbol{\theta}}\tilde{\mathcal{R}}_{\text{reg}}(\boldsymbol{\theta}) &= 0 \\
\lambda\boldsymbol{\theta} + \boldsymbol{H}(\boldsymbol{\theta} - \hat{\boldsymbol{\theta}}) &= 0 \\
(\boldsymbol{H} + \lambda\boldsymbol{I})\boldsymbol{\theta} &= \boldsymbol{H}\hat{\boldsymbol{\theta}} \\
\hat{\boldsymbol{\theta}}_{\text{ridge}} &= (\boldsymbol{H} + \lambda\boldsymbol{I})^{-1}\boldsymbol{H}\hat{\boldsymbol{\theta}}
\end{aligned}$$

We see: minimizer of $L2$-regularized version is (approximately!) transformation of minimizer of the unpenalized version.
Doesn't matter whether the model is an LM – or something else!

GEOMETRIC ANALYSIS OF $L2$ REGULARIZATION / 3

- As λ approaches 0, the regularized solution $\hat{\theta}_{\text{ridge}}$ approaches $\hat{\theta}$. What happens as λ grows?
- Because $\boldsymbol{H}$ is a real symmetric matrix, it can be decomposed as $\boldsymbol{H} = \boldsymbol{Q}\Sigma\boldsymbol{Q}^\top$, where Σ is a diagonal matrix of eigenvalues and $\boldsymbol{Q}$ is an orthonormal basis of eigenvectors.
- Rewriting the transformation formula with this:

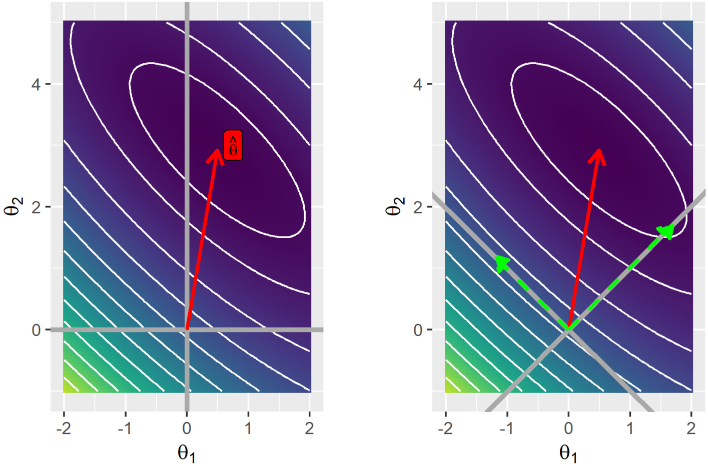
$$
\begin{aligned}
\hat{\theta}_{\text{ridge}} &= \left(\boldsymbol{Q}\Sigma\boldsymbol{Q}^\top + \lambda\boldsymbol{I}\right)^{-1}\boldsymbol{Q}\Sigma\boldsymbol{Q}^\top\hat{\theta} \\
&= \left[\boldsymbol{Q}(\Sigma + \lambda\boldsymbol{I})\boldsymbol{Q}^\top\right]^{-1}\boldsymbol{Q}\Sigma\boldsymbol{Q}^\top\hat{\theta} \\
&= \boldsymbol{Q}(\Sigma + \lambda\boldsymbol{I})^{-1}\Sigma\boldsymbol{Q}^\top\hat{\theta}
\end{aligned}
$$

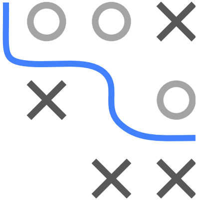
- So: We rescale $\hat{\theta}$ along axes defined by eigenvectors of $\boldsymbol{H}$. The component of $\hat{\theta}$ that is associated with the j-th eigenvector of $\boldsymbol{H}$ is rescaled by factor of $\frac{\sigma_j}{\sigma_j+\lambda}$, where σ_j is eigenvalue.

GEOMETRIC ANALYSIS OF $L2$ REGULARIZATION / 4

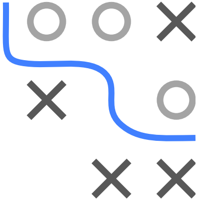
First, $\hat{\boldsymbol{\theta}}$ is rotated by $\boldsymbol{Q}^\top$, which we can interpret as projection of $\hat{\boldsymbol{\theta}}$ on rotated coord system defined by principal directions of $\boldsymbol{H}$:

GEOMETRIC ANALYSIS OF *L*2 REGULARIZATION / 5

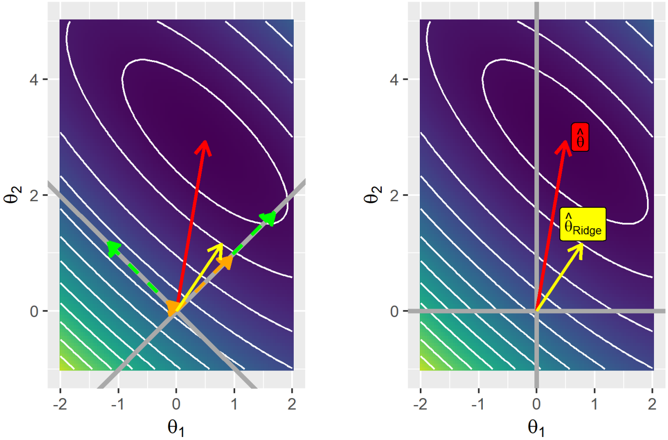




GEOMETRIC ANALYSIS OF $L2$ REGULARIZATION / 6



j-th (new) axis is rescaled by $\frac{\sigma_j}{\sigma_j+\lambda}$ before we rotate back.



GEOMETRIC ANALYSIS OF *L*2 REGULARIZATION / 7

- Decay: $\frac{\sigma_j}{\sigma_j+\lambda}$
- Along directions where eigenvals of $\boldsymbol{H}$ are relatively large, e.g., $\sigma_j >> \lambda$, effect of regularization is small.
- Components / directions with $\sigma_j << \lambda$ are strongly shrunken.
- So: Directions along which parameters contribute strongly to objective are preserved relatively intact.
- In other directions, small eigenvalue of Hessian means that moving in this direction will not decrease objective much. For such unimportant directions, corresponding components of $\boldsymbol{\theta}$ are decayed away.